HPV Test Plan
For

1,3,5–tris(3,5-di-tert-butyl-4-hydroxybenzyl)-1,3,5-triazine-2,4,6 (1H,3H,5H) -trione

CAS No. 27676-62-6

Rubber and Plastic Additives Panel of
The American Chemistry Council

July 11, 2003

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Executive Summary

1,3,5–tris(3,5-di-tert-butyl-4-hydroxybenzyl)-1,3,5-triazine-2,4,6 (1H,3H,5H)-trione (CAS number 27676-62-6) is a chemical intermediate used as a stabilizer for organic substrates such as polymers, synthetic fibers, elastomers, adhesives, waxes, oils and fats. It protects these substrates against thermo-oxidative degradation and contributes to their light stability.

The available data are sufficient to meet the requirements of the High Production Volume (HPV) challenge program with the exception of the developmental toxicity endpoint. A study following Organization for Economic Cooperation and Development (OECD) protocol 414 (Teratogenicity) is proposed.

A. Introduction

An important objective of EPA's HPV chemical challenge program is the gathering and public release of basic hazard information on those chemicals manufactured at high volumes in the United States. The Rubber and Plastic Additives (RAPA) Panel of the American Chemistry Council is participating in this program as a sponsor of this and 35 other compounds, and hereby submits for review and public comment the available data and test plan for 1,3,5–tris(3,5-di-tert-butyl-4-hydroxybenzyl)-1,3,5-triazine-2,4,6 (1H,3H,5H)-trione.

This submission for CAS number 27676-62-6 constitutes a partial revision of documents previously submitted to the Program by the RAPA Panel. In the previous submission, dated December 18, 2001, CAS number 27676-62-6 was included in a category called "Hindered Phenols." In comments dated December 5, 2002, EPA noted that "*the data provided by the sponsor support the category with respect to the physicochemical, environmental fate and ecotoxicological properties of these substances; the health endpoints are less well supported*." Comments received from Environmental Defense (dated May 23, 2002) also noted questions about the "Hindered Phenols" as a category. Accordingly, revised Test Plans and Robust Summaries for the eight chemicals that comprised the former "Hindered Phenols" category will be submitted as two categories (Styrenated Phenols and Bridged Alkyl Phenols), plus two stand-alone chemicals (CAS numbers 68610-51-5 and 27676-62-6).

The RAPA Panel consists of the following member companies: Alco Chemicals; Bayer Corporation; Ciba Specialty Chemicals Corporation; Crompton Corporation; Eliokem, Inc.; Flexsys America L.P.; The Goodyear Tire & Rubber Company; The Lubrizol Corporation; Noveon, Inc.; and, R.T. Vanderbilt Company, Inc.

B. General Substance Information

Chemical Name: 1,3,5–tris(3,5-di-tert-butyl-4-hydroxybenzyl)-1,3,5-triazine-2,4,6 (1H,3H,5H)-trione

Appearance: White to off-white powder

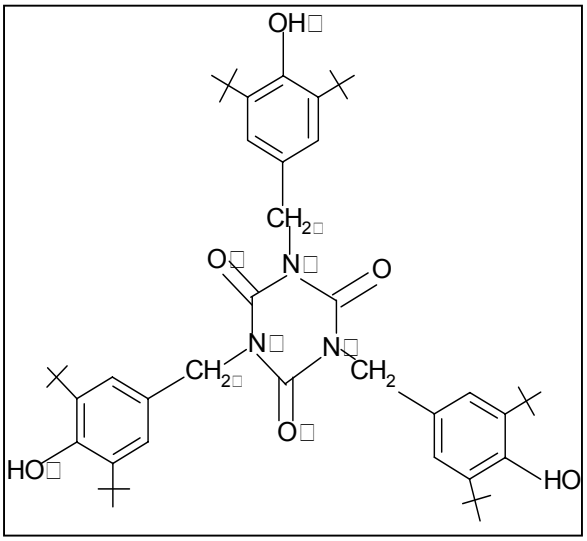
Chemical Abstract Service Registry Number: CAS # 27676-62-6

Common Name / Trade Name: Irganox 3114

Chemical Formula: $C_{48}H_{69}N_3O_6$

Molecular Weight: 784

Structure:



C. General Use Information

1,3,5–tris(3,5-di-tert-butyl-4-hydroxybenzyl)-1,3,5-triazine-2,4,6 (1H,3H,5H)-trione is a sterically hindered phenolic antioxidant. The compound is a chemical intermediate used as a stabilizer for organic substrates such as polymers, synthetic fibers, elastomers, adhesives, waxes, oils and fats. It protects these substrates against thermo-oxidative degradation and contributes to their light stability.

This product has been approved by the U.S. Food and Drug Administration (FDA) for use in various polymers and adhesives intended for food contact applications [21 CFR § 178.2010 and 175.105].

Sales of the product are to industrial users. The polymer industry has an established safety record with such additives and worker exposures are considered minimal. Industrial hygiene programs and Responsible Care® practices are the norm throughout the industry and experience has shown that users handle such products in a careful and conscientious manner. Material Safety Data Sheets (MSDS) are distributed that present detailed hazard data and provide directions for safe handling.

The product can be used in polyolefins, namely polyethylene, polypropylene, polybutene as well as other polymers such as styrene homo- and co-polymers. It may also be used in

linear polyesters, PVC, polyamides and polyurethanes, elastomers such as SBS, EPR, EPDM, and other synthetic rubbers, adhesives, natural and synthetic tackifier resins and other organic substrates. In polyolefins, the concentration levels range typically between 0.05% and 0.3% depending on substrate, processing conditions and long-term thermal stability requirements. The optimum level is application specific.

This compound has good compatibility with most substrates, high resistance to extraction and low volatility. It is odorless and stable when exposed to light. The product can be used in combination with other additives such as costabilizers, light stabilizers and other functional stabilizers. After incorporation in the polymer matrix, it is relatively immobile and release-exposure to humans or the environment is considered minimal.

D. Environmental Endpoints

Existing ecotoxicology data for CAS number 27676-62-6 indicate that there is low concern for acute toxicity to fish, aquatic plants and aquatic invertebrates. The data indicate that the material is not readily biodegradable, however, environmental exposures are expected to be relatively negligible and a low potential for bioaccumulation is indicated. Aquatic toxicology experimental data are available on acute fish toxicity, acute invertebrate toxicity, and alga toxicity for this chemical.

E. Toxicology Endpoints

Available mammalian acute toxicity data indicate very low toxicity by oral and dermal exposure. The LD_{50} values are >5000 mg/kg bw (oral) and >2000 mg/kg bw (dermal). The material does not show mutagenic or clastogenic properties. In sub-chronic toxicity studies in the rat and dog only minor effects have been observed. The substance was found to be neither carcinogenic nor a reproductive toxicant.

F. Conclusions

The available data are sufficient to meet the requirements of the HPV challenge program with the exception of developmental toxicity. A study following OECD protocol 414 (Teratogenicity) is proposed.

1,3,5–tris(3,5-di-tert-butyl-4-hydroxybenzyl)-1,3,5-triazine-2,4,6 (1H,3H,5H) -trione

CAS No. 27676-62-6

SUMMARY TABLE

CAS No. 27676-62-6 PHYSICAL/CHEMICAL ELEMENTS	DATE	RESULTS	FULFILLS REQUIREMENT
Melting Point	2002	219.5-225.5 °C	Yes
Boiling Point	2001	960.98 °C	Yes
Vapor Pressure	2002	5×10^{-15} mm Hg	Yes
Partition Coefficient	2002	log P > 6.0	Yes
Water Solubility	2002	< 1 ppm	Yes
ENVIRONMENTAL FATE ELEMENTS			
Photodegradation	2001	For reaction with hydroxyl radical, predicted rate constant = 66.5×10^{12} cm^3/molecule-sec predicted half-life = 1.93 h	Yes
Stability in Water	2001	Hydrolysis rate extremely slow	Yes
Fugacity	2001	Predicted distribution using Level III fugacity model Air 0.02 % Water 1.15 % Soil 38.4 % Sediment 60.4 % Persistence = 6.4×10^3 h	Yes
Biodegradation	1985	Not biodegradable 0 -7 % after 28 days	Yes
Bioaccumulation	2001	Estimated log BCF = 0.50 (BCF = 3.16)	
ECOTOXICITY ELEMENTS			
Acute Toxicity to Fish	1988	Zebra fish (Brachydanio rerio): LC_{50} (24 – 96 h) => 100 mg/L	Yes
Toxicity to Aquatic Plants	1992	Green algae (Scenedesmus subspicatus): EC_{50} (0 – 72 h) => 100 mg/L NOEC (0 – 72 h) = 33 mg/L	Yes
Acute Toxicity to Aquatic Invertebrates	1988	Daphnia magna: EC_0 (24 h) = > 100 mg/L EC_{50} (24 h) = 32 mg/L EC_{100} (24 h) => 100 mg/L	Yes

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SUMMARY TABLE (CONTINUED)

CAS No. 27676-62-6 HEALTH ELEMENTS	DATE	RESULTS	FULFILLS REQUIREMENT
Acute Toxicity	1986	Rat: LD_{50} (Oral) > 5000 mg/kg	Yes
	1992	Rabbit: LD_{50} (Dermal) > 2000 mg/kg	Yes
Genetic Toxicity in vivo	1987	Chinese hamster: Nonmutagenic in somatic mutation assay (exposed by gavage 5000 mg/kg)	Yes
Genetic Toxicity in vitro	1986	Salmonella typhimurium: No increase in mutations with or without metabolic activation (at doses of 20 – 5000 µg/0.1 mL)	Yes
	1978	Salmonella typhimurium: No increase in mutations with or without metabolic activation (at doses of 25 – 2025 µg/0.1 mL)	Yes
Genetic Toxicity in vitro (non-bacterial)	1991	Chinese hamster V79 cells: No increase in mutations with or without metabolic activation (at doses of 27.5 – 550 µg/0.1 mL)	Yes
Cytogenetic test	1991	Chinese hamster ovary cells: No clastogenic effects	Yes
Repeated Dose Toxicity	1990	Albino Rats: NOEL = 3000 ppm (males) NOEL = 800 ppm (females) (90 days exposure, diet)	Yes
	1970	Albino Rats: NOEL = 10,000 ppm (92-93 days exposure, diet)	
	1970	Dog: NOEL = 10,000 ppm (90 days exposure, diet)	
Developmental Toxicity	NA	NA	Study proposed – OECD 414
Toxicity to Reproduction	1970	90-day repeat dose studies provide appropriate data on reproductive organs	Yes
Chronic Toxicity / Carcinogenicity	1978	2 year rat study: Not carcinogenic at 100 ppm	Yes